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CHAPTER 1

Introduction

1.1 Protoplanetary disk evolution

The universe is an entity in which everything seems to be in motion. The birthplace of our solar system is no exception to this general principle. Planet Earth formed ~ 4.57 billion years ago out of a rotating protoplanetary disk. Together with the other planets and celestial bodies in our solar system, it has been rotating around the sun ever since. The study of protoplanetary disks aims to characterize the evolution of disks towards mature planetary systems such as our solar system. This thesis aims to contribute to our understanding of protoplanetary disk evolution. It focuses on gas and dust in protoplanetary disks around intermediate mass stars (stars which are $\sim 2 - 10$ times more massive than the sun). These objects are also known as Herbig stars, named after their discoverer, George Herbig (1920 – 2013).

The objective of this thesis is tracing the structure and evolution of protoplanetary disks through the infrared emission of dust and gas. In the next sections of this introduction, the general properties of protoplanetary disks are reviewed. The basic tools used in the study of disks are discussed: observations from telescopes and physical models. Thereafter the topics covered in this thesis are discussed: the geometry of protoplanetary disks, ionization of polycyclic aromatic hydrocarbons (PAHs), and the location of forsterite dust in the disk. The introduction ends with a brief outlook on some of the next key questions in the context of this thesis.

1.1.1 Why do we study protoplanetary disks?

In the past decades, discoveries of exoplanets around other stars have ignited a revolution in astronomy. As turned out, not only our own sun, but also other stars have planets orbiting around them. Finding exoplanets is not an easy task. Planets are very small and are fainter than their central star. However, clever observation techniques have overcome these problem and have been, and continue to be, successful in finding new exoplanets. To date, more than thousand exoplanets have been found¹. Based on extrapolations of these observations, it is predicted that billions of exoplanets may reside in our galaxy (Howard et al., 2010). Even exoplanetary atmospheres are currently being investigated. The new era of exoplanetary science enables scientists to answer numerous questions. What kind of exoplanets do we see? Are there any other habitable exoplanets like Earth? How do planets form? Answering these big questions takes patience and requires joint efforts of many scientists working in different disciplines like astronomy, physics, chemistry and computer sciences. To this end, important insights can be obtained by zooming in on one of the earliest phases of the formation of planetary systems: the *protoplanetary disk*.

1.1.2 From clouds, to protoplanetary disks, to planetary systems

The formation of a star and a planetary system starts with a giant cloud consisting of gas, more complex molecules, and dust. An example, of such a cloud is the Orion nebula (Figure 1.1), in which stars and planets are currently forming. When the gravity of (fragments of) the cloud exceeds the supporting gas pressure, the cloud starts to collapse and the material slowly falls to the center. However, since the cloud has some initial rotation, it carries angular momentum. Because angular momentum is a conserved quantity, the angular velocity of the material will increase during infall. As a result, not all the gas and dust can directly fall on the central star because the material is rotating too fast. For that reason, a protoplanetary disk is formed. Eventually, the material in the protoplanetary disk may clump together to form planets. Characterizing this planet formation process is currently one of the main challenges in the study of protoplanetary disks.

Protoplanetary disks are round and are often observed to be $\sim 5 - 10$ times larger than our solar system (see Williams & Cieza 2011 for a review of the properties of protoplanetary disks). Atomic gas, molecules and dust particles are the major observable constituents that build up the disk. Estimates of disk masses range between $\sim 10^{-4} - 10^{-1} M_{\odot}$. For comparison, the cumulative mass of all the planets in our solar system is $1.3 \times 10^{-3} M_{\odot}$. Thus, a fraction of the material in the disk may be expected to clump together into planets. The rest of the mass is either accreted onto the central star or is repelled from the system by other mechanisms such as outflows and jets (see right panel of Figure 1.1).

¹NASA exoplanet archive: <http://exoplanetarchive.ipac.caltech.edu/>

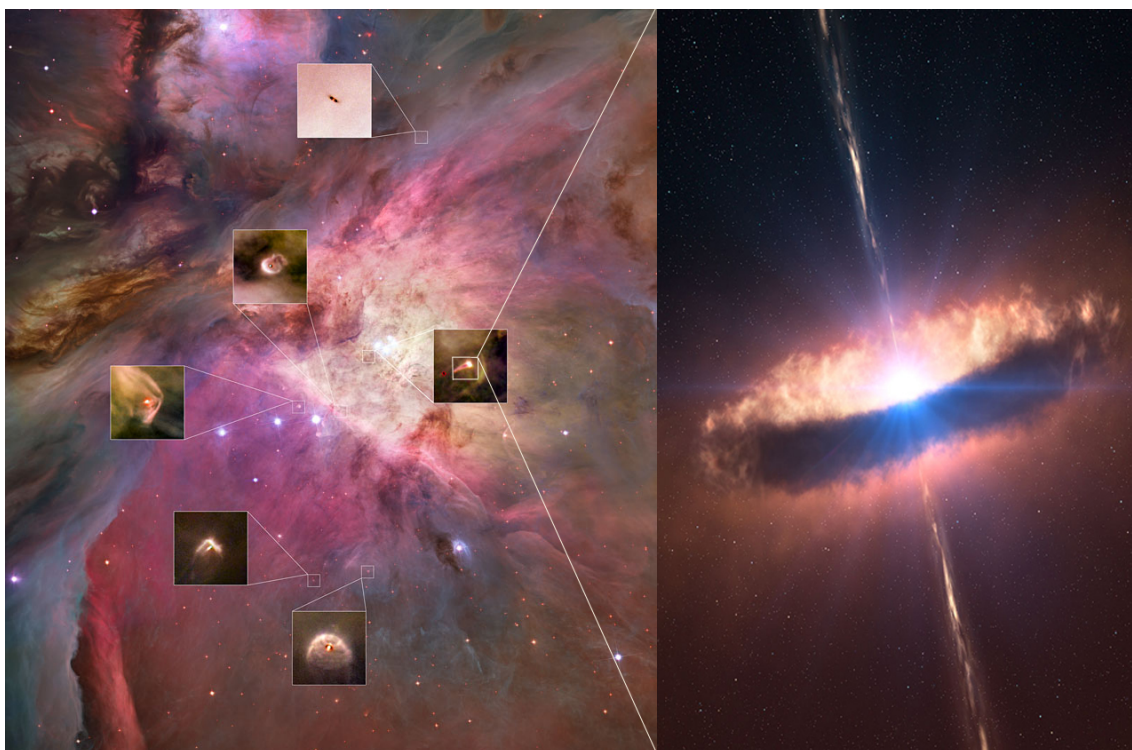


Figure 1.1: *Left:* Hubble telescope image of the Orion nebula. Inside this cloud of gas and dust, hundreds of new stars are born. This image highlights several ‘proplyds’, in which protoplanetary disks can be detected as dark silhouettes in the center of excited material. Credits: NASA, ESA, M. Robberto (Space Telescope Science Institute/ESA), the Hubble Space Telescope Orion Treasury Project Team and L. Ricci (ESO) **Right:** Artist impression of a protoplanetary disk rotating around the star. In roughly 10 million years, the material in the disk can either clump together to form planets, it can be accreted onto the central star, or it can be blown out by outflows and jets as shown by the streams perpendicular to the disk. Credit: ESO/L. Calcada/M. Kornmesser

Modeling protoplanetary disks is essential for the interpretation of telescope observations. A great leap forward came when Shakura & Sunyaev (1973) proposed a recipe to describe the inward transfer of accreting material and outward transfer of angular momentum in a disk. These authors found an analytical model to describe the basic physical structure of a steady state accretion disk. When the Infrared Astronomical Satellite (IRAS) telescope began to observe protoplanetary disks at mid- to far-infrared wavelengths, it was quickly realized that the outer parts of the disk were producing more emission than what was expected for flat disks (Adams et al., 1987). Kenyon & Hartmann (1987) suggested that the gas and dust in planetary disks are actually in hydrostatic equilibrium (i.e. the density in the disk is set by an equilibrium between the pressure of the gas and the vertical component of the stellar gravity). Because the temperature gradient and the gradient of stellar gravity are both decreasing towards larger distances from the star, their interplay results in a flaring disk structure (i.e. a thicker disk outward). This explanation was further improved by Chiang & Goldreich (1997) and has become standard in state of the art disk models. A sketch of a flaring disk is shown in Figure 1.2.

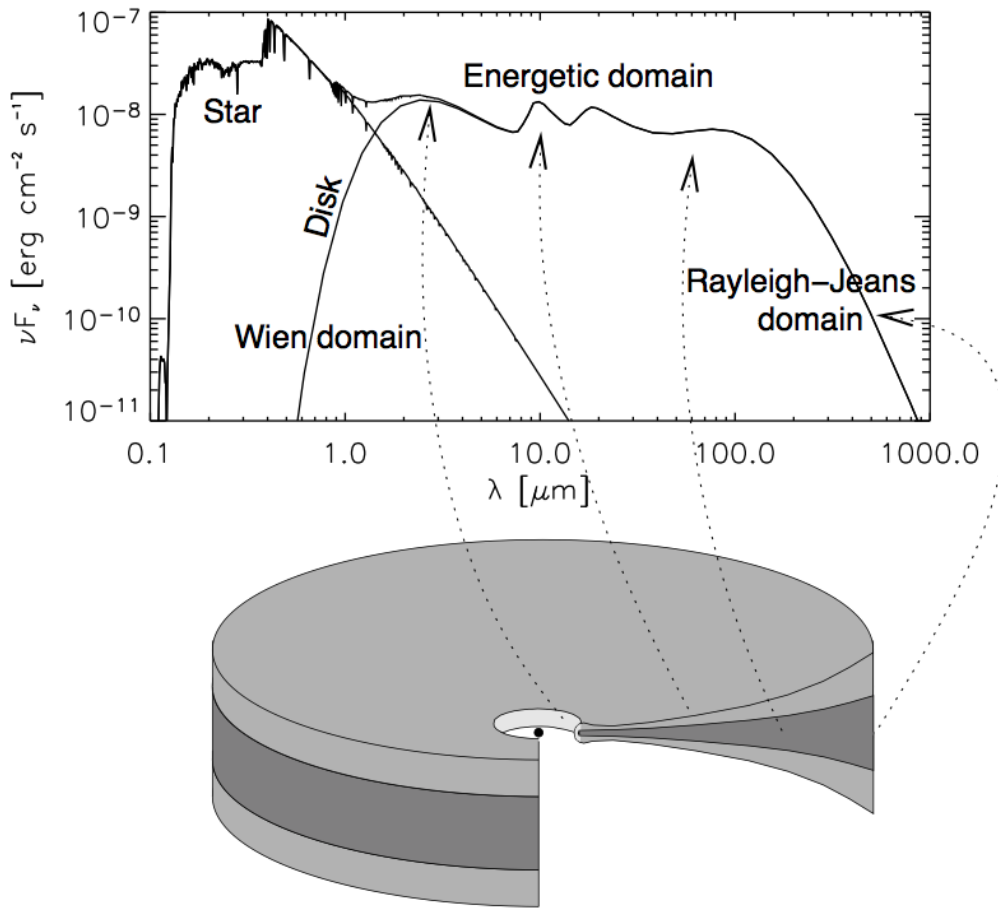


Figure 1.2: A sketch of a flaring protoplanetary disk (Dullemond et al., 2007b). The central star dominates the emission (expressed in the flux quantity νF_ν) at optical wavelengths ($\lambda \lesssim 1 \mu\text{m}$). The inner disk ($T \sim 1500 \text{ K}$) can be traced at near-infrared wavelengths ($1 \lesssim \lambda \lesssim 5 \mu\text{m}$). The surface of the disk ($T \sim 100 - 500 \text{ K}$) is best studied at mid-infrared wavelengths ($5 \lesssim \lambda \lesssim 50 \mu\text{m}$). The colder ($T \lesssim 100 \text{ K}$) outer parts of the disk are traced though observations in the far-infrared up to millimetre wavelengths ($\lambda \gtrsim 50 \mu\text{m}$). Not shown on this SED is that accretion columns and/or accretion spots on the star can have temperatures of $\sim 10^4 \text{ K}$ or more leading to an excess at ultraviolet wavelengths.

Studies of disks around young stars in clusters suggested that most stars lose their disk in ~ 10 million years (e.g. Mamajek 2009). This means that compared to the total lifetime of the star (~ 10 billion years for a sun-like star), the evolution of the disk is a rapid process. Turbulent motions inside protoplanetary disks may induce planet formation (Weidenschilling, 1980). Due to these motions, small dust particles collide, stick together, grow to larger planetesimals and eventually may form planets with sizes similar to the Earth. When the planet grows to even larger sizes, it becomes so massive that it starts accreting gas from the disk and transforms into a gas giant such as Jupiter. This scenario

is known as the core-accretion scenario (Pollack et al., 1996). Evidence for this planet formation process can be found by carefully analyzing the emission we observe from the disks. If the system is close enough, then the disk may be spatially resolved and structures can potentially reveal disk processes. Figure 1.2 shows how we can trace different parts of the disk by observing at different wavelengths. This flux versus wavelength diagram is known as the spectral energy distribution (SED) and displays the total emission per wavelength, which trace different parts of the disks. The emission we observe from the star and the disk shows up on an SED. In this thesis, the SED is used as an important diagnostic tool to study the evolution of disks.

1.1.3 Disk evolution: self-shadowed and transitional disks

A general picture of disk evolution of protoplanetary disks is shown in figure 1.3. It starts as a massive flaring disk, and through evolutionary processes such as grain growth, grain settling and planet formation, the disk eventually transforms into a debris disk. In this thesis it is proposed that in this evolutionary sequence, two types of protoplanetary disks represent the most important disk structures observed in the sample of Herbig stars: self shadowed (‘flat’) disks and transitional (‘flaring’) disks. Note that it is yet unknown whether transitional disks form out of self-shadowed disks, or that both disks types represent independent pathways of disk evolution.

Self-shadowed disks are thought to have a disk geometry which is high (puffed up) close to the star but flatter outwards. A typical SED shows strong near-infrared excess, but little emission at far-infrared wavelengths. Among Herbig stars, the SED types were identified as groups by Meeus et al. (2001). An interpretation of their disk structure quickly followed. Dullemond & Dominik (2004a,b, 2005) proposed that the flatness of the outer disk was the result of dust particles which stick together and grow in size. If the dust grains become more massive, they settle down to the mid-plane and the disk becomes flatter. Another important factor is that the inner disk is believed to ‘puff up’ because it receives a relatively large amount of stellar radiation at the inner edge of the disk (Dullemond et al., 2001). The increase of the inner disk temperature causes the inner disk to increase its vertical scaleheight. As a result, the thick inner disk casts a shadow which decreases the emission from the outer disk.

The second subclass consist of the transitional disks (e.g. Calvet et al. 2005). These protoplanetary disks have a smaller excess at near-infrared wavelengths, but still significant excess at longer wavelengths (Strom et al., 1989). These types of disks are characterized by large, empty regions, depleted of gas and dust. These empty regions are called ‘gaps’ and have a ring like (i.e., annular) shape. As an example, Figure 1.4 shows the transitional disk of HD 169142 (studied in detail in Chapter 2). If the gap is located close to the star, it is also known as an ‘inner hole’. It is widely believed that these gaps are a result of the formation of planets. When all the material in the disk at a certain radius from the star is being accreted onto a planet, a gap is formed in the disk (e.g., Armitage 2011).

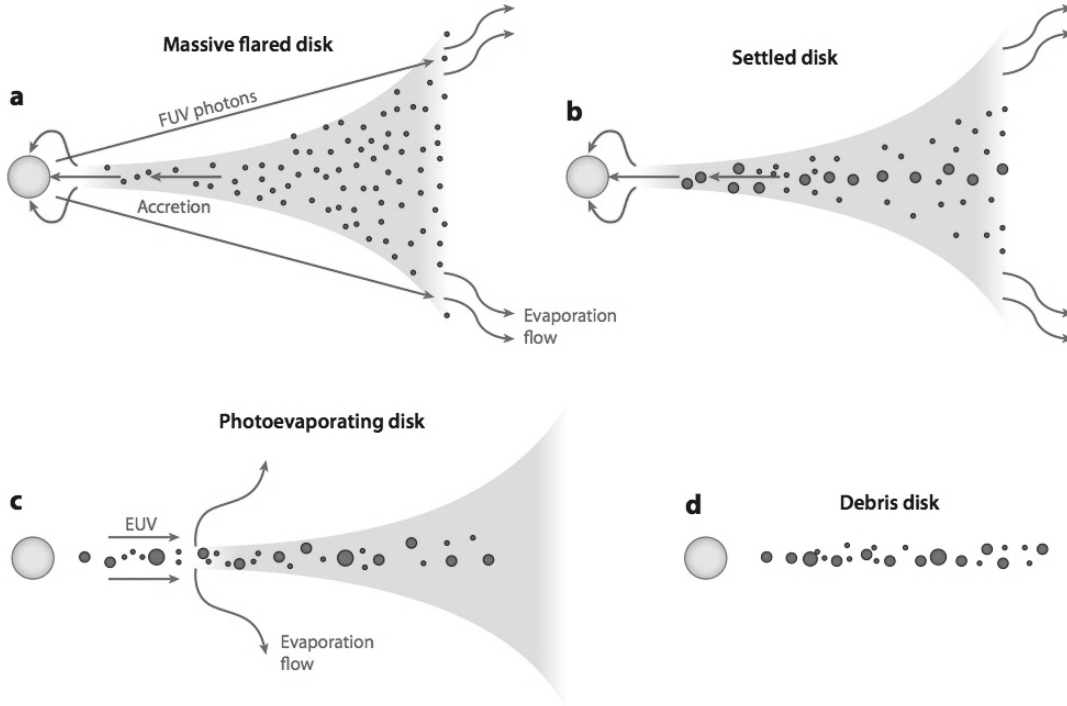


Figure 1.3: This sketch shows several processes in the evolution of a typical disk. **(a)** A massive flaring disk early in its evolution. The disk loses mass through accretion onto the star and photoevaporation of the outer disk. **(b)** A flat, self-shadowed disk. Grains grow into larger bodies that settle to the mid-plane of the disk. **(c)** A transitional disk. As the disk mass and accretion rate decrease, the outer disk no longer replenishes the inner disk. Material in the inner disk sticks together to form planets, or photoevaporation removes all material by radiation pressure. **(d)** The debris disk, which has a very low mass and is not always detectable. The small grains are removed by radiation pressure and Poynting-Robertson drag. Only large grains, planetesimals, and/or planets are left. Figure adapted from Williams & Cieza (2011).

There are also physical mechanisms, other than planet formation, that are responsible for the evolution of disks. For example, photo-evaporation by high energetic UV and X-ray emission can also create gaps and inner holes (e.g. Alexander et al. 2006, Gorti et al. 2009). Together with mechanisms such as viscous accretion by the magneto-rotational instability (e.g. Hartmann et al. 1998, Chiang & Murray-Clay 2007), and dynamical interactions between the disk and stellar or substellar companions (Artymowicz & Lubow, 1994), physical processes in the disk may be responsible for a variety of observational appearances of the protoplanetary disk. Disentangling their effects is a challenging task and requires both analytic models as well as high spectral and spatial resolution observations.

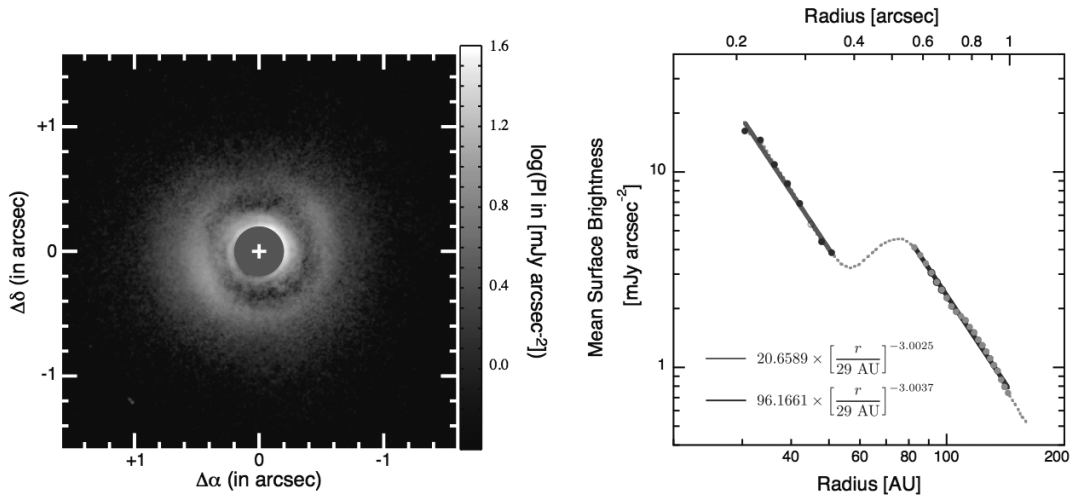


Figure 1.4: Left: the polarized intensity image of the transitional disk around HD 169142 observed pole-on in the H-band ($\lambda \sim 1.6 \mu\text{m}$) with Subaru/HiCIAO (Momose et al., 2013). A large empty ring (i.e. a ‘gap’) can be seen between $\sim 60 - 80$ AU. Right: the averaged radial distribution of the intensity. The disk structure of HD 169142 is studied in Chapter 2.

1.2 Observations and models of protoplanetary disks

Stars with protoplanetary disks reveal themselves through electromagnetic radiation from X-ray up to millimetre wavelengths. To be able to understand how disks evolve, a combination of observations from high quality telescopes and analytic and numerical models is required. This thesis uses observations of state-of-the-art infrared telescopes. In particular observations from the Spitzer and Herschel space telescopes are an important observational input for this thesis. We now briefly discuss a short history and future prospects of space based infrared observatories.

1.2.1 New generations of telescopes

New insights in astronomy are often the result of new generations of telescopes. In 1983, the Infrared Astronomical Satellite (IRAS) was the first space telescope to perform a survey of the entire sky at infrared wavelengths (Figure 1.5). IRAS triggered the first systematic studies on the variety of SEDs of protoplanetary disks. Follow-up space based infrared telescopes further opened up of the infrared sky, improving in spatial and spectral resolution and sensitivity. In 1995, the Infrared Space Observatory (ISO) was the first to reveal the incredible richness of the mid-IR spectrum. Most notably, the characteristic emission features from polycyclic aromatic hydrocarbon and silicate dust grains could be studied in detail. The analysis of these spectral features provides insight into the physical processes in disks. Less than a decade later, ISO was followed up in 2003 by the Spitzer Space Observatory. Spitzer improved the infrared view of protoplanetary disks



Figure 1.5: Six generations of space based infrared telescopes. New telescopes often improve spatial resolution, spectral resolution and sensitivity. Top, from left to right: the Infrared Astronomical Satellite (IRAS) launched in 1983, the Infrared Space Observatory (ISO) launched in 1995 and the Spitzer Space Observatory launched in 2003. Bottom, from left to right: the Herschel space telescope launched in 2009, and the James Webb Space Telescope (JWST), with a proposed launch in 2018 and the Space Infrared Telescope for Cosmology and Astrophysics (SPICA), with a proposed launch in 2025.

with unprecedented sensitivity and became the first telescope to directly capture the infrared light from extrasolar planets: the ‘hot Jupiters’ TrES-1 (Charbonneau et al., 2005) and HD 209458b (Ballester et al., 2007). On May, 14, 2009, the next space telescope was launched towards its operational orbit: Herschel. Three instruments on board of Herschel performed imaging photometry and spectroscopy in the far-infrared and sub-millimeter part of the spectrum (55–672 μm). Herschel provided the spectral resolution and sensitivity to study the spectral features at 69 μm from crystallised silicate dust grain called forsterite. The James Webb Space Telescope (JWST) and the Space Infrared Telescope for Cosmology and Astrophysics (SPICA) are the next telescopes capable of observing at infrared wavelengths, and are scheduled to be launched in 2018 and 2025 respectively. JWST and SPICA have even larger mirrors and more sensitive instruments which will provide unprecedented resolution and sensitivity from the near- to far-infrared.

Space based telescopes have the advantage that they do not suffer from atmospheric absorption (especially at wavelengths above $\lambda \sim 1 \mu\text{m}$) and turbulence. However, their mirror sizes are limited to a few meter because they require expensive rockets to launch them into space. Another disadvantage is their limited life-time: infrared space observatories typically only last for a couple of years due to depletion of the cooling system. Ground based telescopes can be made much larger and are easier to maintain. The world

today counts hundreds of professional ground-based telescopes. Obviously, the bigger the better. Examples of impressive telescopes which are currently the most important deliverers of protoplanetary disk observations are the Subaru telescope on Mauna Kea in Hawaii, and the Very Large Telescope (VLT) and the Atacama Large Millimeter/submillimeter Array (ALMA), both in the Atacama Desert of northern Chili.

New telescopes often improve observations in three ways: the spatial resolution, the spectral resolution and the sensitivity. A higher spatial resolution enables the telescope to zoom in and observe smaller structures. A better spectral resolution allows telescopes to better observe emission profiles of gas lines and substructure in solid state features. Finally, if the instrument has a higher sensitivity, a telescope can observe in a shorter time, fainter objects, often located at greater distances in space, with a better signal to noise. For this thesis, all three dimensions are important. Chapters 2, 3 and 4 present high spatial resolution images taken at 18.8 and 24.5 μm from the Subaru, VLT and Gemini North and South telescopes. Chapter 5 presents a detailed study of sensitive PAH features, with a high signal to noise ratio, for a large sample of Herbig stars. In Chapter 6 the improved spectral resolution of the Herschel space telescope is used to analyze the spectral shape of the forsterite 69 μm feature.

1.2.2 From observations to physical models

It is important to understand the physical processes which are responsible for the radiation emitted by the materials around young stars. The most relevant emission processes in disks are from the interaction of stellar light with atomic gas, molecules and dust.

For atomic and molecular gas, the interaction with incident energy carriers (i.e. such as photons from the central star or energetic particles like cosmic rays) can produce strong emission lines at specific wavelengths. The wavelengths of these emission lines are defined by internal energy transitions, either discretely or continuously distributed over energy. Furthermore, the emission is influenced by macroscopic properties such as the density (i.e. pressure, surface, volume, number of particles and temperature). Groups of atoms can build up molecules which are more complex in terms of their structure and their emission spectrum. Simple molecules such as CO have ro-vibrational band structures that can be resolved with very high spectral resolution spectrographs. At some size, molecules start to behave partly like a solid (surface) in that they show band structure. Because internal rotational and vibrational modes between the atoms in the molecule can result in emission features which are blended. This generates so-called emission feature complexes. An example of such features are the mid-infrared emission profiles of very large molecules such as the PAHs.

In protoplanetary disks, the absorption at mid-infrared wavelengths is dominated by dust grains. Silicate dust grains dominate the radiation in the low energy regime. The thermal emission profile of silicate dust as a function of wavelength is characterised by the temperature and the material properties such as size and composition. In this way, the characteristic mid-infrared spectral features of silicate grains have important diagnostic value for constraining properties like the chemical composition and sizes of dust grains.

Comparing telescope observations to analytic and numerical models is essential to provide a quantitative interpretation. Ideally, a model is as simple as possible, though the level of complexity often grows as the resolution of the observations increases. Whether observations are needed to test the model, or vice versa, depends on the nature of the scientist. An example of a very simple disk model is one that assumes that the SED of a disk can be fitted by a distribution of blackbodies within a certain temperature range. While this model may give a relatively good fit to the SED, it fails to explain the underlying physics (i.e. the structure of the disk). Thus, more realistic models involve detailed particle properties, radiative transfer, chemical descriptions and more complex physics to understand and predict observations. The analysis of protoplanetary disks must include a computational code which can follow the photon paths in disks and produce model images and SEDs which are used to compare to the observations. Throughout this thesis, this has been done using the Monte Carlo radiative transfer code MCMax (Min et al., 2009).

1.3 Topics in this thesis

In the next sections, it is discussed how in this thesis observations and models are combined to give a better understanding of the structure and evolution of protoplanetary disks. The infrared emission of dust and gas are considered: amorphous silicate dust grains to trace the structure of the disk, neutral versus ionized PAHs in gas flows through the gap, and crystalline dust (forsterite) in the inner and outer regions of protoplanetary disks.

1.3.1 Emission from dust grains around disk gaps

Dust grains provide the material from which terrestrial planets and the cores of the giant planets (in the core accretion model) are made. In the diffuse interstellar medium (ISM), dust is mainly composed of silicates with sizes $\sim 0.1 \mu\text{m}$ (Draine, 2003). During the evolution from the ISM to protoplanetary disks to planets, dust undergoes significant processing. Molecules freeze out from the gas phase onto dust grain surfaces and form icy mantles (Bergin & Tafalla, 2007). Dust grains stick together and grow and thereby become more massive and settle down to the mid-plane of the disk (Dullemond & Dominik, 2004a, 2005). Small dust grains are replenished in the disk by fragmentation processes. The dust size distribution in the disk is therefore determined by a complex balance between dust coagulation and fragmentation (Dullemond & Dominik, 2008). To study the disk geometry and composition we need to understand the observational appearance of the silicates grains in the disk: a class of materials also commonly found on Earth (i.e. 90 % of the Earths crust consists of silicates).

1.3.1.1 Imaging the geometry of the disk

Silicate dust particles are the dominant absorbers and scatterers in disks and re-radiate stellar light in the $1 \mu\text{m}$ to 1mm range. Amorphous silicates are easily identified through

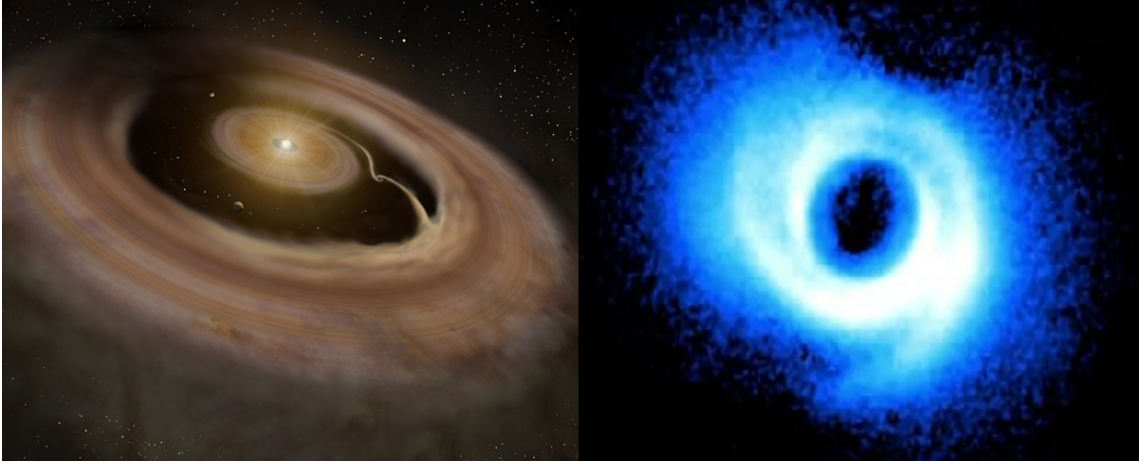


Figure 1.6: Left: artist impression of a transitional disk. A stream of material is flowing inward through the gap, accreting onto the planet, and replenishing the inner disk. Credit: The Graduate University for Advanced Studies, Japan. Right: Subaru/HiCIAO observations of the transitional disk HD 135344 B (Muto et al., 2012). Obvious spiral arms can be seen in this disk.

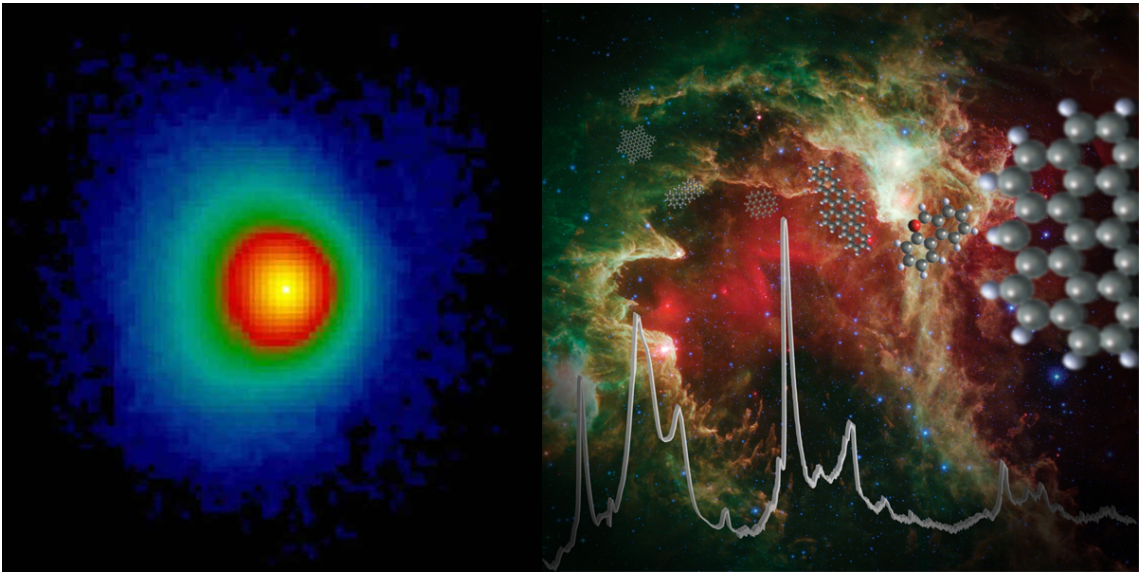


Figure 1.7: Left: HD 97048 observed by VLT/VISIR in the PAH filter (Lagage et al., 2006). The PAHs on the surface of the disk emit at mid-infrared wavelengths, and the disk surface can be traced. Right: an interstellar nebula showing the emission from PAHs in red. Over plotted are some PAH molecular structures and a typical interstellar PAH infrared spectrum.

broad spectral bands at 10 and 18 μm (see e.g. Henning 2010 for a review on cosmic silicates). Because the temperature of the dust decreases with the distance from the central star, different wavelengths trace different disk radii. As gaps form, possibly due to planet formation, a decrease of radiation is detected in both the SED and in resolved images. Another effect of the formation of a disk gap is that the vertical wall (i.e. the inner edge of the outer disk) is now exposed to the star and increases in brightness because it receives the emission which would otherwise fall on the disk. Depending on the location (i.e. temperature range) and size of the gap in the disk, the gap may be identified in the SED. A typical gap can be seen in the SED by a decreased emission dip at wavelengths corresponding to the temperature range where the gap is residing. This dip is directly followed by an increase of emission at longer wavelengths, originating from the wall of the outer disk.

An SED can be used as an indirect indicator of the presence of a disk gap. However, an SED is inconclusive in determining the location of the disk gap because the temperature of the inner edge of the outer disk also depends on the luminosity of the star, the grain properties and the opaqueness of the inner disk structure. By imaging protoplanetary disks with high spatial resolution, it is possible to lift this degeneracy, directly observe disk gaps, and thereby constrain the radius of the gap. In addition, with sufficient spatial resolution, it is also possible to observe the structures of the material around the gap such as banana shapes (e.g. in HD 142527, Fujiwara et al. 2006, Casassus et al. 2013) and spiral arms (e.g. in HD 135344 B, Muto et al. 2012, Figure 1.6).

1.3.2 Emission from polycyclic aromatic hydrocarbons

Many astrophysical objects show a rich spectrum of infrared emission features associated with polycyclic aromatic hydrocarbons (PAHs, Leger & Puget 1984, Allamandola et al. 1985). With respect to their size, PAHs can be considered as gas. However, their opacities and broad emission features are more characteristic of dust. They exchange charge in collisions with the gas and can break up or release some subgroups if they interact with energetic radiation. PAH features are ubiquitous in space, for example in H II regions, reflection nebulae, young stellar objects, planetary nebulae, post-asymptotic giant branch objects, nuclei of galaxies, and ultra-luminous infrared galaxies (Tielens 2008 and references therein). Peeters et al. (2002) classified PAH emission profiles in three different classes based on the positions of their feature centers, class A: representing interstellar material illuminated by a star, such as HII regions, reflection nebulae, and the general ISM of the Milky Way and other galaxies, class B: sources associated with circumstellar material and include PNe and a variety of post-AGB objects, and Herbig AeBe stars, and class C: a few extreme carbon-rich post-AGB objects. This classification appears to be tracing the extent to which PAH molecules have been processed by their environments, particularly the stellar radiation field. PAHs in disks have been used to trace the disk structure. Observations presented by Lagage et al. (2006) and Doucet et al. (2006) demonstrated that PAH emission can be used to derive the flaring angle of the disk of HD 97048 (Figure 1.7, left). Figure 1.7 (right) shows a composite image of PAH emission in an interstellar nebula, the structure of some PAH molecules, and a typical infrared PAH

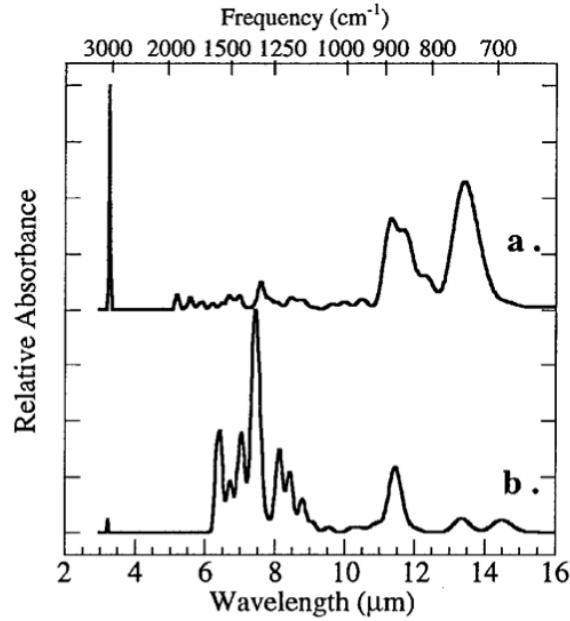


Figure 1.8: The absorption spectrum produced by neutral PAHs (top) compared with the spectrum produced by the same PAHs but ionized (bottom). The ionization state has a strong effect on the relative intensities (Allamandola et al., 1989).

spectrum. PAHs account for a significant part of all cosmic carbon (Snow & Witt, 1995, Puget & Leger, 1989, Allamandola et al., 1989). They have been detected in cometary material during the Deep Impact mission (Lisse et al., 2006) and were brought back to Earth by the Stardust mission (Sandford et al., 2006). It is therefore believed that carbon bearing species such as PAHs are also important constituents of planets in habitable zones (Kasting et al., 1993).

1.3.2.1 PAH ionization

Nearly 50% of Herbig Ae/Be stars have strong PAH emission (e.g. Meeus et al. 2001, Acke & van den Ancker 2004). A variety of PAH emission intensities and ionization fractions have been found (Sloan et al., 2005, Boersma et al., 2008). The ionization balance is predominantly set by the incident UV radiation field, which ionizes the PAHs, and the density of electrons, which can recombine with the PAHs to their neutral state. The peak ratio of the $I_{6.2}/I_{11.3}$ μm PAH features can be used as a measure for the ratio of neutral versus ionized PAH (Allamandola et al. 1989, see Figure 1.8). Ionized PAHs have a higher $I_{6.2}/I_{11.3}$ μm ratio, whereas neutral PAHs emit stronger in the 11.3 band.

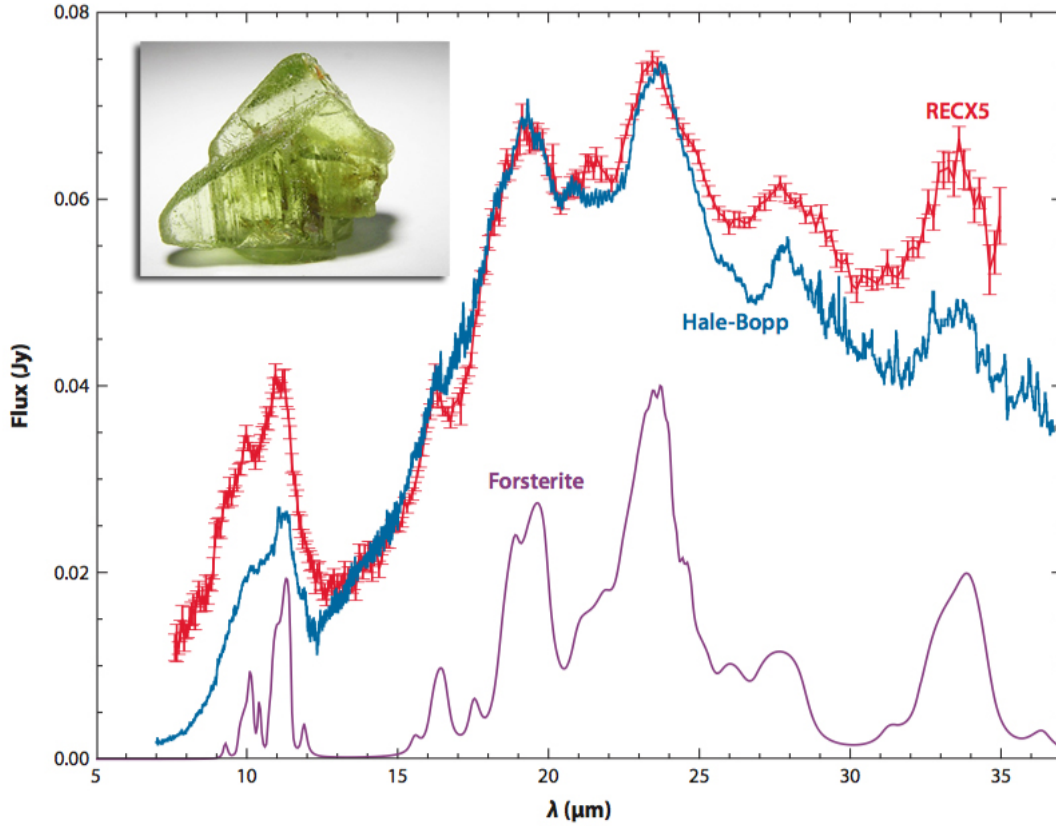


Figure 1.9: This figure shows the striking similarity between a laboratory forsterite spectrum and the spectrum from the comet Hale-Bopp and the spectrum from the proto-planetary disk RECXS. On the upper right corner a figure is shown of a forsterite rock. Figure adopted from Henning (2010).

1.3.3 Emission from forsterite grains

In the ISO spectra of Herbig Ae/Be systems, dust species such as silicates, both crystalline as well as amorphous, metallic iron, iron oxide, carbonaceous grains and water ice, have been identified (e.g. Malfait et al. 1998, Bouwman et al. 2000). Since dust in the ISM is largely amorphous (Kemper et al., 2004), substantial dust processing takes place in the protoplanetary disks surrounding protostars. At high temperatures ($T \gtrsim 1000$ K), forsterite is formed by condensation from the gas phase or by thermal annealing of amorphous silicates. The crystallisation products are mainly enstatite and forsterite, producing stronger and narrower features. They have the same chemical composition as the amorphous silicates. However, their atoms are ordered in a lattice with long range order. The emission features at about 10 and 18 μm , correspond to Si–O stretching and O–Si–O bending vibrations respectively. The 69 μm feature can be attributed to translational motions of the metal cations and complex translations involving metal and Si atoms. Forsterite shows narrower spectral features which carry information of the chemical composition as well as the grain size (Figure 1.9). By comparing the mid-infrared spectra

with laboratory spectra of dust material (e.g. Koike et al. 2003, 2006, Suto et al. 2006), the individual dust species can be identified. With observations from the ISO, Spitzer and Herschel telescopes, enormous progress has been made in determining both the dust composition as well as the processes that govern this composition in protoplanetary disks.

1.3.3.1 The forsterite 69 μm feature

The most recent insights in the characteristics of forsterite are made possible by observations from the Herschel space telescope. Information about the temperature, grain size and iron fraction can be derived from the shape of the 69 μm feature. The forsterite 69 μm feature has been observed and analysed by Sturm et al. (2010), Mulders et al. (2011) and Sturm et al. (2013). The widths and peak positions of the 69 μm detections indicate low temperature (~ 200 K) forsterite. This indicates that forsterite must be located at regions where it is significantly colder as compared to the location where they are formed ($T \gtrsim 1000\text{K}$). This is consistent with earlier analysis of forsterite in protoplanetary disks by Bouwman et al. (2008), Juhász et al. (2010). Either efficient radial mixing from warmer regions in the inner disk, or in situ formation by a local process such as shocks or parent body processing must be responsible.

1.4 Outline of this thesis

The study of protoplanetary disks is ‘in motion’. The work in this thesis spans over a timescale of four years, and already during these years, many new insights of protoplanetary disks have been presented. This thesis aims to contribute to the key question ‘How do planets form?’. It focuses on the characterisation of several elements in the earliest phases of planet formation in protoplanetary disks: the connection between the SED and disk gaps (Chapters 2, 3 and 4), PAHs in the gas flows in disk gaps (Chapter 5) and dust processing of forsterite in evolving protoplanetary disks (Chapter 6).

In Chapters 2, 3 and 4, Q-band ($\lambda = 18.8 \mu\text{m}$ and $\lambda = 24.5 \mu\text{m}$) observations have been analysed using the radiative transfer code MCMax to constrain the location of the gap. Sizes of the large gaps are identified in the transitional objects HD 97048, HD 169142, HD 135344 B, Oph IRS 48, HD 34282 and HD 100453. None of these objects show broad amorphous silicate features in the SED. By using direct imaging we confirm the presence of gaps in the disks and constrain their location. The main conclusion is therefore that the absence of the silicate feature can be used as a tracer of large size gaps in the temperature regime $\sim 200 - 500$ K. A second conclusion is that almost all flaring disks, within the sample of well known Herbig stars, are actually transitional disks. It thus seems that there are distinct ways in which disk can evolve: from flaring to flat disks (by grain growth and settling), from flaring to transitional disks (likely due to the formation of planets), or a combination of both: from flaring to flat to transitional.

In Chapter 5 an analysis is presented of the ionization balance of PAHs in Herbig stars. An analytic model for the ionization balance of PAHs is implemented in the radiative transfer code MCMax. The model was applied to four key objects for which spatial information was available about the location of PAHs in the disk. It is found that the PAHs are ionized when they are located in the gas flows through protoplanetary disk gaps. This is because in the low density, optically thin disk gaps, the local UV field is high, while the electron density is low. It is found that PAHs in the high density, optically thick disks are neutral, independent of the distance to the central star. The main conclusion is therefore that the band strength ratio $I_{6.2}/I_{11.3}$ can be used as a tracer of gas flows through protoplanetary disk gaps.

The analysis of forsterite spectra from disks must include radiative transfer models to properly study the influence of the disk geometry and different radial distributions of forsterite grains in the disk. In addition, optical depth effects can be taken into account. In Chapter 6 all the Herbig stars of which the 69 μm wavelength domain have been observed by Herschel/PACS are studied. The consistency between the forsterite features in the Spitzer/IRS and Herschel/PACS spectra are tested. For all objects, independent estimates of the forsterite temperature are made using the I_{23}/I_{69} feature ratio and the shape of the 69 μm feature. For the evolved transitional objects HD 141569 and Oph IRS 48, it is found that the 69 μm features may indicate larger grain sizes. This could be a result of substantial grain processing. The non-detections and general weakness of the 69 μm feature in flat disks indicate that the forsterite temperature is high ($T \gtrsim 300$ K). The location of the forsterite in these types of disks must be close to the star. This is consistent with the hypothesis that radial mixing is not very efficient in flat disks. This may be connected with the flatness of the disk, which can be a sign of low turbulence.

1.5 Future outlook

The final answers to many key questions are still ahead of us. And of course, as soon as they have been answered, they will be replaced by new questions. In the study of protoplanetary disk towards planetary systems, an important role will be taken by new generations of telescopes. ALMA has just started to explore the millimetre sky with great spatial resolution and sensitivity. And with the JWST and SPICA on their way, the future of infrared astronomy may be expected to boost again. In the context of this thesis, there are several relevant science questions waiting to be further explored:

- Is the emission from PAHs in disk gaps of Herbig stars indeed largely ionized? Will JWST be able to confirm this prediction?
- What is the influence of PAHs on heating and cooling events in the disk gaps? How are other gas/molecule diagnostics sensitive for the PAHs? The PAHs have a strong effect of the photoelectric heating in the disk. However, the interaction between the PAHs and the other material in the disk must be studied in more detail. This will allow us to understand whether the observational variety of PAH spectral signatures are a consequence of the disk structure, and vice versa.

- How radially extended are flat disks? The high sensitivity of ALMA is needed to observe the outer regions of flat disks. In addition, is there a relation between the mid-infrared (MIR) spectral index $F_{30}/F_{13.5}$ (i.e. the degree of self-shadowing, Acke et al. 2009) and the mm luminosity for flat disks? If grains in flat disks continue to drift inwards, where they accrete onto the star, and thus make the disk ‘small and fat’, the disk gets smaller over time. This may be indicated by the disk sizes of HD 163296 and HD 31648 which are several hundreds of AU in size and have high mm luminosities, while the disk of HD 104237 is only ~ 70 AU large and has a much lower mm luminosity.
- Are flat disks precursors of transitional disks? If a planet would form in a flat disk, could it increase the scale-height of the grains in the outer disk (e.g., increase the turbulence), and/or are small grains from inner disk blown outward and do they ‘land’ on the outer disk? A modeling study could investigate such scenarios.
- What are the differences between Herbig and T Tauri objects? We can study the influence of stellar properties on the disks by comparing full disks and transitional disks of T Tauri and Herbig stars. In this way, the consistency of their gap size characteristics and connection to mid- to far- infrared spectral colors can be studied. Herbig stars are known for their strong near-infrared (NIR) excess as compared to T Tauri stars. Is there a significant difference between the NIR excess of Herbig and T Tauri systems? If so, this may be attributed to the higher ultraviolet (UV) luminosity in Herbig stars. Including stochastically heated VSG in the disk could be examined as a solution. There is a strong correlation between the absence of the silicate feature and the $F_{30}/F_{13.5}$ ratio. Is this correlation also present in T-Tauri objects? In addition, most Herbig Be stars are self-shadowed/flat, while for T Tauri stars, there does not seem to be a clear distinction between full/flat and transitional/flaring disks. Does the mass of the central star influence the structure of the disk?
- Are dust grains within the snow-line (i.e. where the temperature is $\gtrsim 150$ K) significantly smaller? Test models show that the grain population needed to model a typical disk with silicate feature (group Ia) has a much higher abundance of small grains as compared to the grain population needed to fit a typical disk which does not show silicate features (group Ib). Possibly, this may reflect that the coagulation/-fragmentation balance of dust grains in the inner region lies more toward smaller sizes than in the outer disks. Remarkably, the transition between group Ia and Ib seems to be indicated by the presence of small grains above ~ 150 K (Chapter 4). It would be interesting to study whether this is caused by the properties of the grains. Could particles in the outer disk stick together more easily due to icy mantles around the dust grain?
- Can laboratory measurements characterize the broadening of the $69\ \mu\text{m}$ feature width as a function of grain size and low ($\sim 0 - 1\%$) fractions of iron inclusion?

The study of the chemistry and mineralogy inside protoplanetary disks is rapidly advancing. New modeling studies focus on to improve their description of the interaction

between the gas, the molecules and the dust in protoplanetary disks. New observations of dusty grains and ices originating in protoplanetary disks will gain further insights on the physical processes that alter the chemical composition and sizes of the grains in the disk. Perhaps we may soon find a better understanding between the variety of chondrites found in and around Earth, and the physical formation history of our solar system. With many new telescopes approaching, and excellent collaborations made between scientists all over the world, the future of exoplanetary science looks promising.